

2,4,6-Cycloheptatrien-1-one, 2-amino-

Other names:	2-Aminotropone 2-Amino-2,4,6-cycloheptatriene-1-one 2-Amino-2,4,6-cycloheptatrien-1-one
Inchi:	InChI=1S/C7H7NO/c8-6-4-2-1-3-5-7(6)9/h1-5H,(H2,8,9)
InchiKey:	PIOPKWFBKZTUMS-UHFFFAOYSA-N
Formula:	C7H7NO
SMILES:	Nc1cccccc1=O
Mol. weight [g/mol]:	121.14
CAS:	6264-93-3

Physical Properties

Property code	Value	Unit	Source
ie	9.43 ± 0.02	eV	NIST Webbook
log10ws	-0.53		Crippen Method
logp	0.629		Crippen Method
mcvol	97.280	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	71.10 ± 0.40	kJ/mol	303.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6264933&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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